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Structural Phase Transition, Electronic and Magnetic Properties of Sr_2FeMoO_6

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The nuclear and magnetic structures of Sr_2FeMoO_6 have been investigated using neutron powder diffraction and Mössbauer spectroscopy at temperatures between 10 and 460 K. Fe and Mo atoms are found to order on alternate sites, as expected, giving rise to a double-perovskite type unit cell. Upon cooling, a structural phase transition from cubic $Fm\bar{3}m$ to tetragonal $I4/m$ occurs at $\sim$400 K. In the tetragonal $I4/m$ structure as the temperature decreases, the FeO_6 and MoO_6 octahedra rotate continuously around the c axis by an angle of up to $\sim 5.6^o$. In the $I4/m$ phase, the magnetic moments for Fe and Mo order ferrimagnetically. The Fe magnetic spins first align along the c direction and then rotate to an angle of $\sim 54^o$ with respect to the c axis; the refined Fe magnetic moment saturates at $\sim 4.3\mu_B$. Mössbauer spectroscopy measurements show that the average valence of Fe is intermediate between the high spin configuration values of Fe^{+2} and Fe^{+3}. The temperature dependence of the mean hyperfine field is in good agreement with the neutron diffraction results and gives the same transition temperature.